

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_Y\Data\VY100124\  
 Data File : VY019746.D  
 Acq On : 01 Oct 2024 17:11  
 Operator : SY/MD  
 Sample : P4225-01  
 Misc : 5.02g/5.0mL/MSVOA\_Y/SOIL/A  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 MSVOA\_Y  
 ClientSampleId :  
 TR-04-092724

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y090924S.M

Title : SW846 8260

Signal : TIC: VY019746.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 2.086       | 51            | 60          | 61           | rBV2     | 5127           | 11796         | 11.60%          | 2.095%        |
| 2         | 2.178       | 73            | 75          | 77           | rBV3     | 1985           | 2131          | 2.10%           | 0.379%        |
| 3         | 2.525       | 131           | 132         | 136          | rVB3     | 1865           | 1668          | 1.64%           | 0.296%        |
| 4         | 2.574       | 136           | 140         | 142          | rVB3     | 1168           | 1402          | 1.38%           | 0.249%        |
| 5         | 2.970       | 202           | 205         | 209          | rVB5     | 903            | 1070          | 1.05%           | 0.190%        |
| 6         | 4.068       | 379           | 385         | 388          | rBV2     | 836            | 1636          | 1.61%           | 0.291%        |
| 7         | 4.671       | 481           | 484         | 488          | rVB5     | 841            | 1394          | 1.37%           | 0.248%        |
| 8         | 4.811       | 502           | 507         | 508          | rBV3     | 1190           | 1232          | 1.21%           | 0.219%        |
| 9         | 4.958       | 526           | 531         | 533          | rBV3     | 961            | 1725          | 1.70%           | 0.306%        |
| 10        | 6.140       | 721           | 725         | 727          | rBV3     | 953            | 1384          | 1.36%           | 0.246%        |
| 11        | 6.220       | 735           | 738         | 740          | rBV2     | 757            | 1018          | 1.00%           | 0.181%        |
| 12        | 6.878       | 838           | 846         | 847          | rBV3     | 2697           | 5194          | 5.11%           | 0.923%        |
| 13        | 6.988       | 862           | 864         | 868          | rVB3     | 946            | 1226          | 1.21%           | 0.218%        |
| 14        | 7.195       | 894           | 898         | 900          | rBV3     | 1003           | 1617          | 1.59%           | 0.287%        |
| 15        | 7.530       | 950           | 953         | 955          | rBV2     | 861            | 1059          | 1.04%           | 0.188%        |
| 16        | 7.634       | 961           | 970         | 976          | rBV      | 14095          | 33096         | 32.55%          | 5.879%        |
| 17        | 7.707       | 976           | 982         | 995          | rVB2     | 28783          | 67426         | 66.31%          | 11.977%       |
| 18        | 7.908       | 1012          | 1015        | 1018         | rBV3     | 728            | 1067          | 1.05%           | 0.190%        |
| 19        | 8.061       | 1030          | 1040        | 1049         | rBV2     | 11857          | 30688         | 30.18%          | 5.451%        |
| 20        | 8.213       | 1062          | 1065        | 1067         | rBV3     | 789            | 1083          | 1.07%           | 0.192%        |
| 21        | 8.542       | 1117          | 1119        | 1122         | rVB2     | 1231           | 1062          | 1.04%           | 0.189%        |
| 22        | 8.616       | 1122          | 1131        | 1140         | rBV2     | 39939          | 85503         | 84.09%          | 15.188%       |
| 23        | 9.061       | 1201          | 1204        | 1206         | rBV2     | 830            | 1069          | 1.05%           | 0.190%        |
| 24        | 9.347       | 1245          | 1251        | 1252         | rBV3     | 811            | 1349          | 1.33%           | 0.240%        |
| 25        | 9.798       | 1320          | 1325        | 1328         | rBV5     | 1017           | 1990          | 1.96%           | 0.353%        |
| 26        | 10.103      | 1368          | 1375        | 1384         | rBV      | 57051          | 101681        | 100.00%         | 18.062%       |
| 27        | 11.109      | 1538          | 1540        | 1543         | rVB3     | 1069           | 1250          | 1.23%           | 0.222%        |
| 28        | 11.146      | 1543          | 1546        | 1549         | rBV5     | 926            | 1170          | 1.15%           | 0.208%        |
| 29        | 11.182      | 1549          | 1552        | 1555         | rBV3     | 1103           | 1804          | 1.77%           | 0.320%        |
| 30        | 11.231      | 1555          | 1560        | 1562         | rBV6     | 684            | 1081          | 1.06%           | 0.192%        |
| 31        | 11.310      | 1572          | 1573        | 1578         | rVB4     | 906            | 1234          | 1.21%           | 0.219%        |
| 32        | 11.414      | 1582          | 1590        | 1601         | rVV      | 43386          | 75129         | 73.89%          | 13.345%       |
| 33        | 11.493      | 1601          | 1603        | 1608         | rVB3     | 939            | 1668          | 1.64%           | 0.296%        |
| 34        | 12.011      | 1685          | 1688        | 1692         | rBV4     | 736            | 1091          | 1.07%           | 0.194%        |
| 35        | 12.304      | 1733          | 1736        | 1739         | rBV3     | 1184           | 1688          | 1.66%           | 0.300%        |
| 36        | 12.402      | 1747          | 1752        | 1759         | rBV      | 24677          | 40531         | 39.86%          | 7.200%        |

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 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 MSVOA\_Y  
 ClientSampleId :  
 TR-04-092724

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y090924S.M  
 Title : SW846 8260

|    |        |      |      |      |      |       |       |        |        |
|----|--------|------|------|------|------|-------|-------|--------|--------|
| 37 | 12.877 | 1824 | 1830 | 1831 | rVV5 | 998   | 1840  | 1.81%  | 0.327% |
| 38 | 12.908 | 1833 | 1835 | 1838 | rVV3 | 797   | 1033  | 1.02%  | 0.183% |
| 39 | 12.938 | 1838 | 1840 | 1846 | rVB6 | 778   | 1044  | 1.03%  | 0.185% |
| 40 | 13.164 | 1875 | 1877 | 1881 | rVB4 | 1122  | 1282  | 1.26%  | 0.228% |
| 41 | 13.340 | 1899 | 1906 | 1913 | rBV2 | 19406 | 32250 | 31.72% | 5.729% |
| 42 | 13.493 | 1928 | 1931 | 1933 | rBV4 | 1056  | 1068  | 1.05%  | 0.190% |
| 43 | 13.603 | 1948 | 1949 | 1953 | rBV4 | 1076  | 1601  | 1.57%  | 0.284% |
| 44 | 13.657 | 1956 | 1958 | 1961 | rVB4 | 1012  | 1223  | 1.20%  | 0.217% |
| 45 | 13.688 | 1961 | 1963 | 1966 | rBV4 | 963   | 1070  | 1.05%  | 0.190% |
| 46 | 13.767 | 1973 | 1976 | 1978 | rBV4 | 1053  | 1356  | 1.33%  | 0.241% |
| 47 | 13.810 | 1980 | 1983 | 1985 | rBV3 | 1039  | 1351  | 1.33%  | 0.240% |
| 48 | 14.115 | 2031 | 2033 | 2037 | rBV5 | 854   | 1223  | 1.20%  | 0.217% |
| 49 | 14.212 | 2046 | 2049 | 2052 | rBV4 | 797   | 1129  | 1.11%  | 0.201% |
| 50 | 14.389 | 2075 | 2078 | 2084 | rVB8 | 1577  | 3035  | 2.98%  | 0.539% |
| 51 | 14.468 | 2089 | 2091 | 2094 | rVB4 | 1400  | 1235  | 1.21%  | 0.219% |
| 52 | 14.877 | 2154 | 2158 | 2160 | rBV3 | 1265  | 1679  | 1.65%  | 0.298% |
| 53 | 14.968 | 2168 | 2173 | 2174 | rBV5 | 1345  | 1754  | 1.73%  | 0.312% |
| 54 | 15.108 | 2194 | 2196 | 2198 | rBV3 | 1271  | 1366  | 1.34%  | 0.243% |
| 55 | 15.273 | 2220 | 2223 | 2225 | rBV3 | 1633  | 2140  | 2.10%  | 0.380% |
| 56 | 15.340 | 2232 | 2234 | 2238 | rVB4 | 1357  | 1415  | 1.39%  | 0.251% |
| 57 | 15.523 | 2259 | 2264 | 2267 | rBV7 | 1277  | 1716  | 1.69%  | 0.305% |
| 58 | 15.694 | 2290 | 2292 | 2295 | rBV4 | 1080  | 1027  | 1.01%  | 0.182% |
| 59 | 15.828 | 2313 | 2314 | 2318 | rBV3 | 1180  | 1192  | 1.17%  | 0.212% |
| 60 | 15.968 | 2335 | 2337 | 2339 | rVB3 | 1653  | 1307  | 1.29%  | 0.232% |
| 61 | 15.992 | 2339 | 2341 | 2344 | rBV4 | 1258  | 2115  | 2.08%  | 0.376% |
| 62 | 16.072 | 2353 | 2354 | 2359 | rVB5 | 1007  | 1383  | 1.36%  | 0.246% |
| 63 | 16.181 | 2370 | 2372 | 2375 | rVB4 | 1307  | 1189  | 1.17%  | 0.211% |
| 64 | 16.437 | 2409 | 2414 | 2415 | rVB4 | 993   | 1294  | 1.27%  | 0.230% |
| 65 | 16.535 | 2425 | 2430 | 2434 | rBV6 | 1051  | 2105  | 2.07%  | 0.374% |
| 66 | 16.742 | 2462 | 2464 | 2467 | rBV4 | 1299  | 1320  | 1.30%  | 0.234% |

Sum of corrected areas: 562954

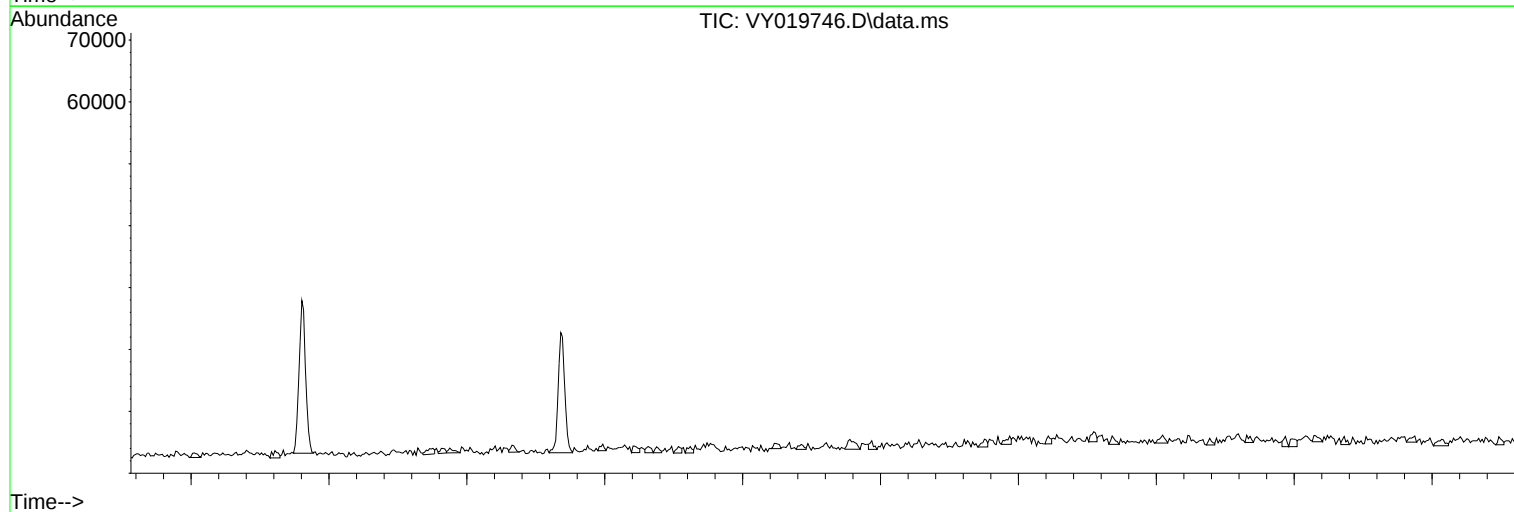
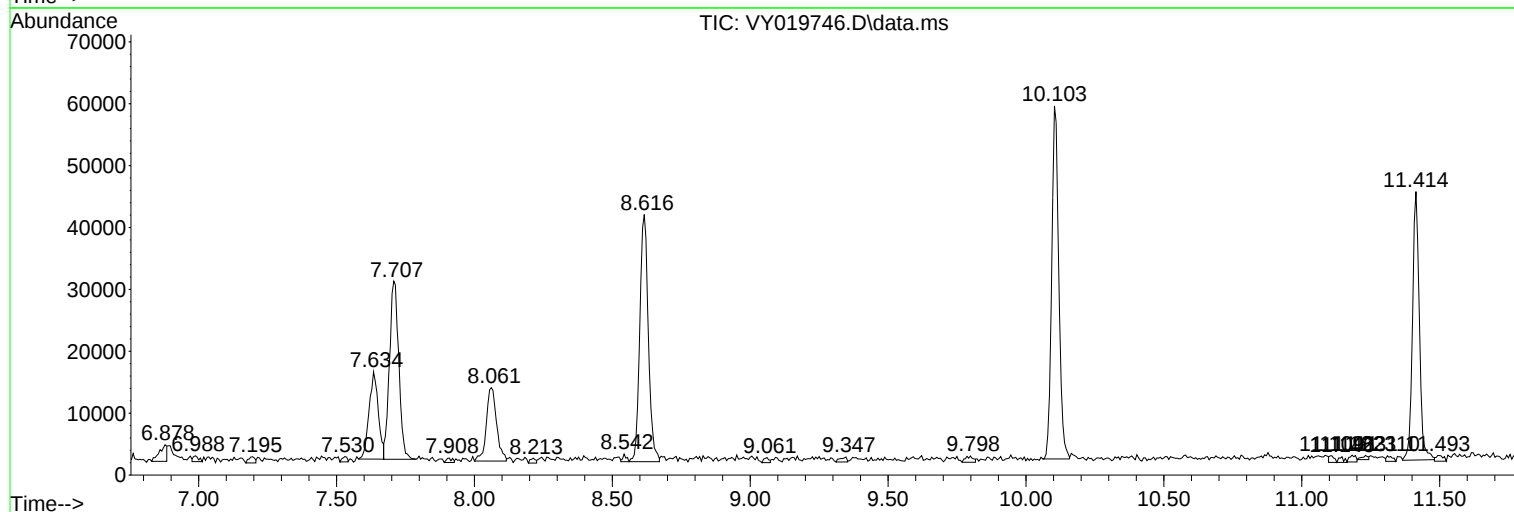
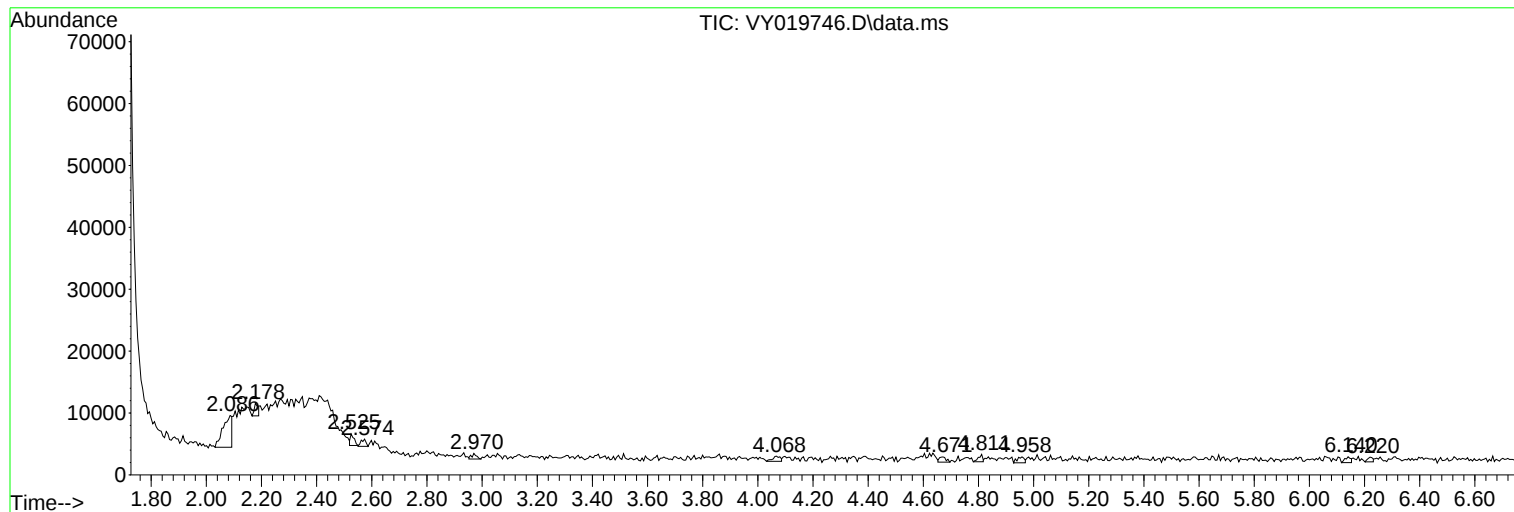
Data Path : Z:\voasrv\HPCHEM1\MSVOA\_Y\Data\VY100124\  
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Instrument :  
MSVOA\_Y  
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TR-04-092724

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y090924S.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_Y\Data\VY100124\  
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Instrument :  
MSVOA\_Y  
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TR-04-092724

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y090924S.M  
Quant Title : SW846 8260

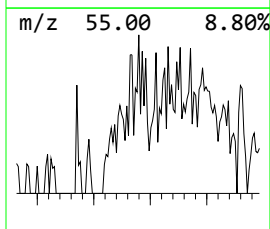
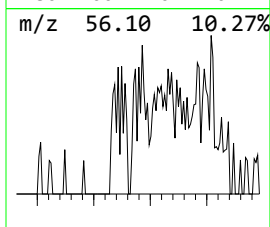
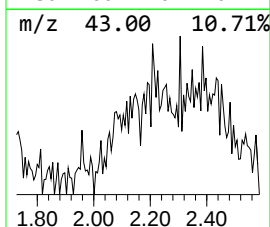
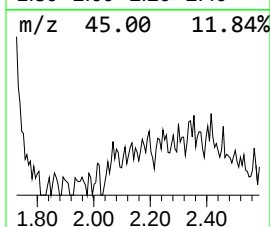
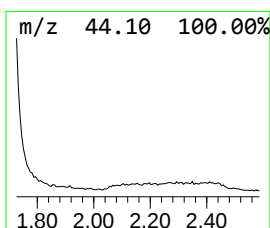
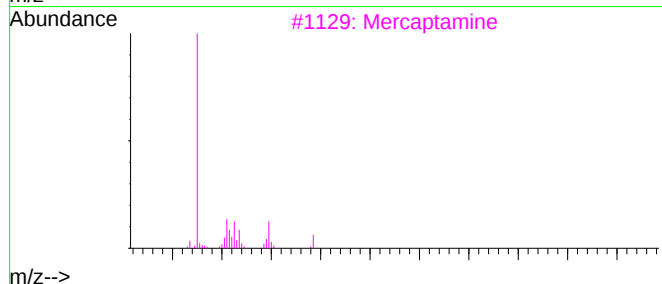
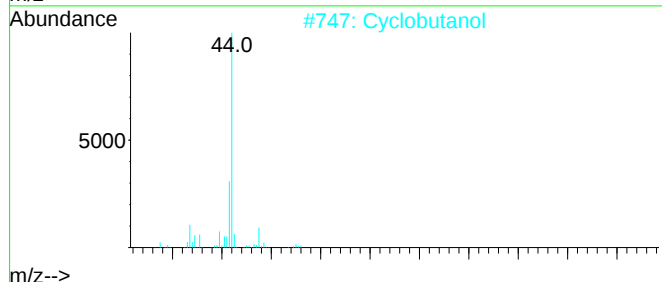
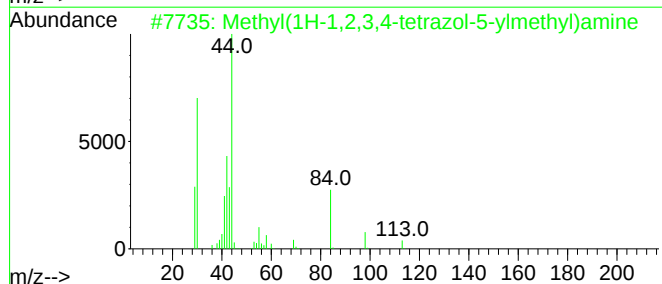
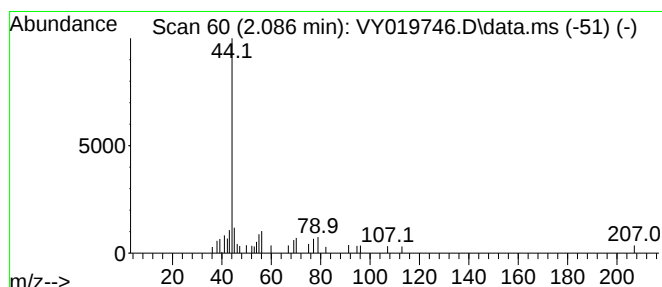
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 1 unknown2.086 Concentration Rank 1

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 2.086 | 8.75 ug/l | 11796 | Pentafluorobenzene | 7.713 |

| Hit# of 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|-----------|-------------------------------------|-----|----------|--------------|------|
| 1         | Methyl(1H-1,2,3,4-tetrazol-5-ylm... | 113 | C3H7N5   | 1000444-24-2 | 36   |
| 2         | Cyclobutanol                        | 72  | C4H8O    | 002919-23-5  | 36   |
| 3         | Mercaptamine                        | 77  | C2H7NS   | 000060-23-1  | 9    |
| 4         | Acetamide, 2,2,2-trifluoro-         | 113 | C2H2F3NO | 000354-38-1  | 9    |
| 5         | Acetic acid, hydroxy[(1-oxo-2-pr... | 145 | C5H7NO4  | 006737-24-2  | 9    |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT    | EstConc | Units | Response | # | RT    | Resp  | Conc |
|------------------|-------|---------|-------|----------|---|-------|-------|------|
| unknown2.086     | 2.086 | 8.8     | ug/l  | 11796    | 1 | 7.713 | 67426 | 50.0 |